Activities and Collaborations

Division of Quantum Condensed Matter Physics

Kazuhiro YABANA

Leader of the Division

Faculty members of Division of Quantum Condensed Matter Physics

Computational Nano-Sciences:

Kenji SHIRAISHI (prof., former group leader -2013; moved to Nagoya Univ.)
Susumu OKADA (prof., -2013; moved to Dept. of Physics, collaborative member)
Jun-Ichi IWATA (lecturer, -2011; moved to Univ. Tokyo)

Computational Optical Sciences:

Kazuhiro YABANA (prof., group leader)
Xiao-Ming TONG (assoc. prof.)
Nobuya MAESHIMA (lecturer)

Strongly-Correlated Systems:

Hiroyasu KOIZUMI (assoc. prof.)

*Currently, open recruitment of one associate professor in the division (deadline 3/31)

*All the members also affiliated to: Graduate School of Pure and Applied Sciences

Computational Nano-Sciences

K. SHIRAISHI (prof., former group leader -2013; moved to Nagoya Univ.)
S. OKADA (prof., -2013; moved to dept. of Physics)
J.-I. IWATA (lecturer, -2011; moved to Univ. Tokyo)

RSDFT code: Large-scale electronic structure calculations

Collaboration between physicists and computer scientists in the Center

Journal of Computational Physics 229 (2010) 2339–2363

Contents lists available at ScienceDirect

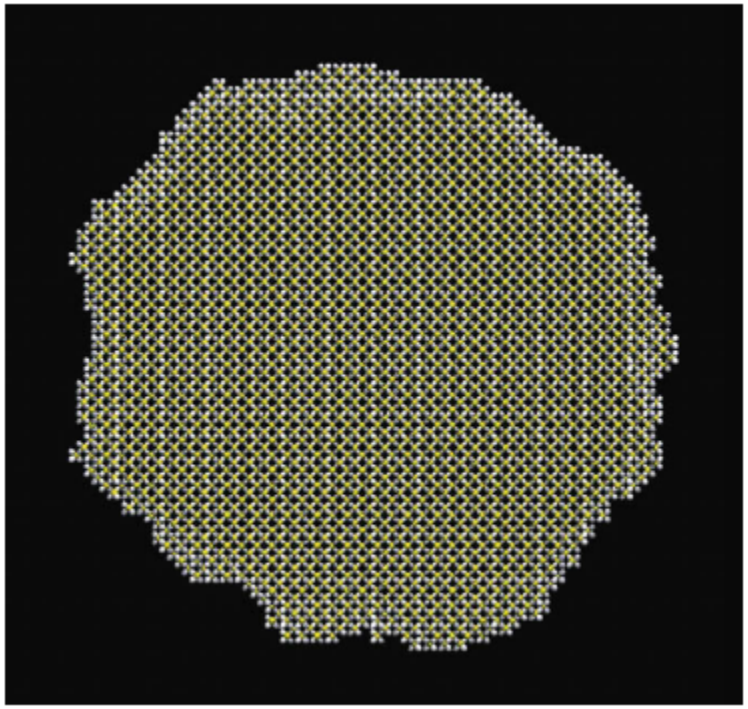
Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

A massively-parallel electronic-structure calculations based on real-space density functional theory

Jun-Ichi Iwata [a,*], Daisuke Takahashi [a], Atsushi Oshiyama [a,b], Taisuke Boku [a], Kenji Shiraishi [a], Susumu Okada [a], Kazuhiro Yabana [a]

[a] Center for Computational Sciences, University of Tsukuba, 1-1-1 Tenoudai, Tsukuba, Ibaraki 305-8577, Japan
[b] Department of Applied Physics, School of Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan



Main developer: Jun-Ichi Iwata, CCS until 2011.7.

In Fig. 17, we show the self-consistent electronic charge density and the atomic configuration of the Si nanowire with surface roughness. Obviously the system has no symmetry. Therefore, the calculation must be performed without any help of symmetry operation which is utilized to reduce the size of the matrix. The model system consists of 14,366 atoms, and the total number of grid points is 4,718,592. The total computational time to obtain the self-consistent electronic-structure was 292 h, including 93 iteration steps, with 1024 nodes of the PACS-CS.

Scaled up at K-computer, collaborations with U. Tokyo, RIKEN, Fujitsu

ACM Gordon Bell Prize, Peak-Performance at SC11

Yukihiro Hasegawa (RIKEN), Junichi Iwata (University of Tokyo), Miwako Tsuji (University of Tsukuba), Daisuke Takahashi (University of Tsukuba), Atsushi Oshiyama (University of Tokyo), Kazuo Minami (RIKEN), Taisuke Boku (University of Tsukuba), Fumiyoshi Shoji (RIKEN), Atsuya Uno (RIKEN), Motoyoshi Kurokawa (RIKEN), Hikaru Inoue (Fujitsu), Ikuo Miyoshi (Fujitsu), and Mitsuo Yokokawa (RIKEN).

Electronic structure calculation of
Silicon nanowire composed of
100,000 Si atoms.
Execution performance of 3.08 petaflops
(execusion efficiency 43.6%)
at K-computer, Kobe.

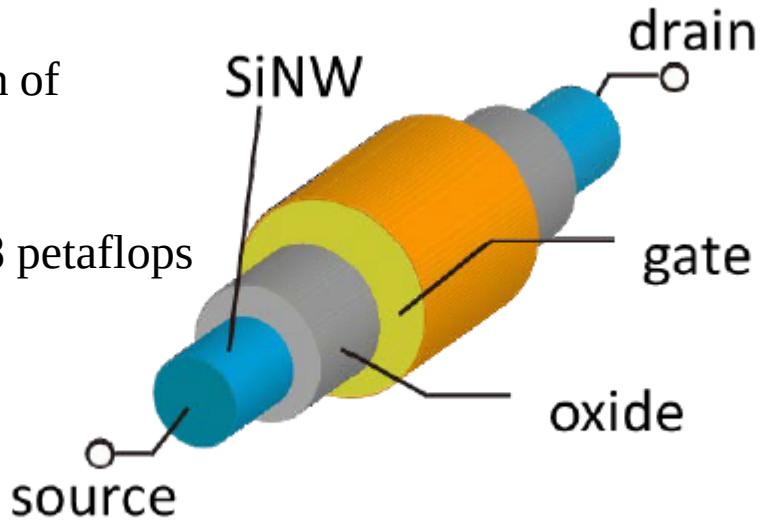
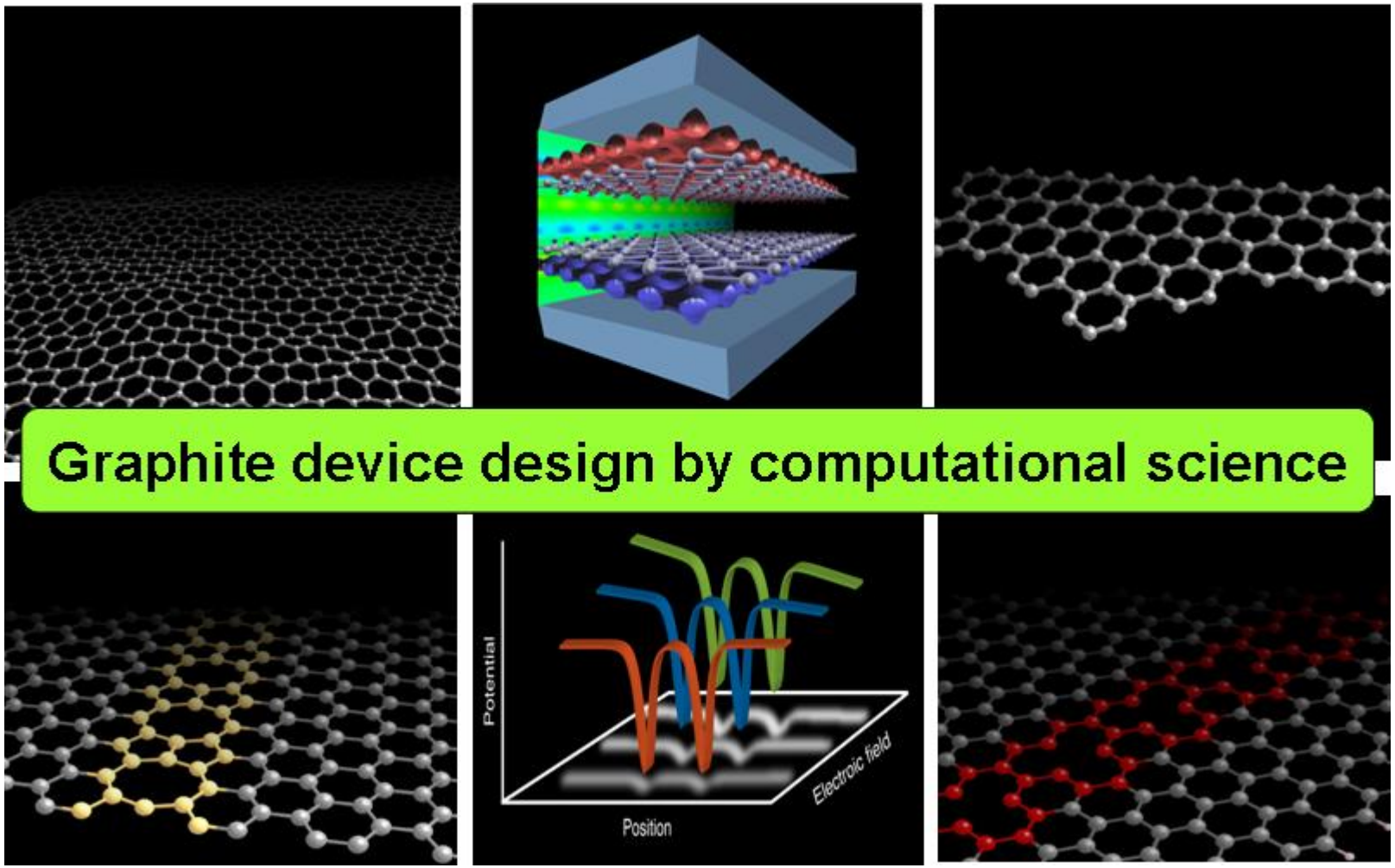


Figure 1: Diagram of a next-generation field effect transistor using a silicon nanowire

First-principles study on graphene

by S. Okada

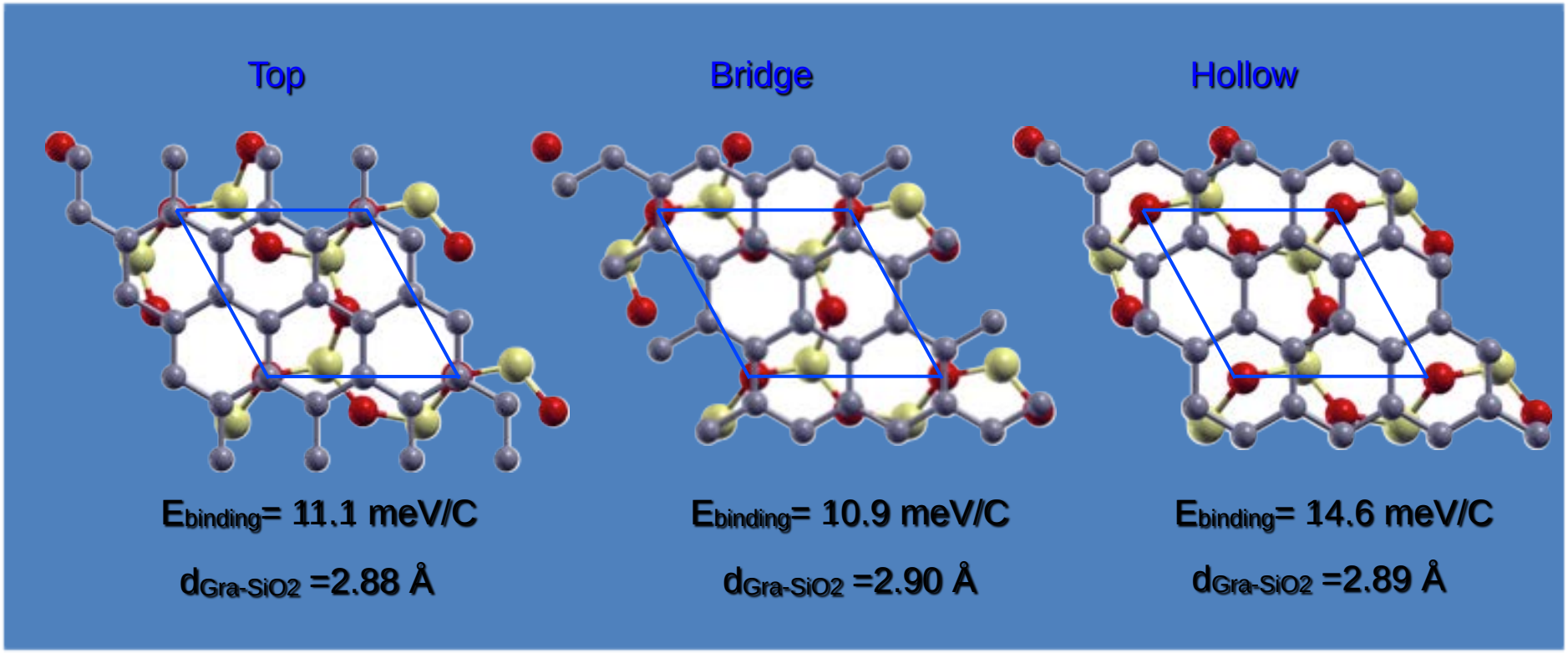


Graphene on O-terminated SiO_2

N. T. Cuong et al. Phys. Rev. Lett. 106, 106801 (2011)

Graphene is a two-dimensional sheet material, a slice of graphite.
Because of its edge part, it behaves like metal and shows magnetic property.

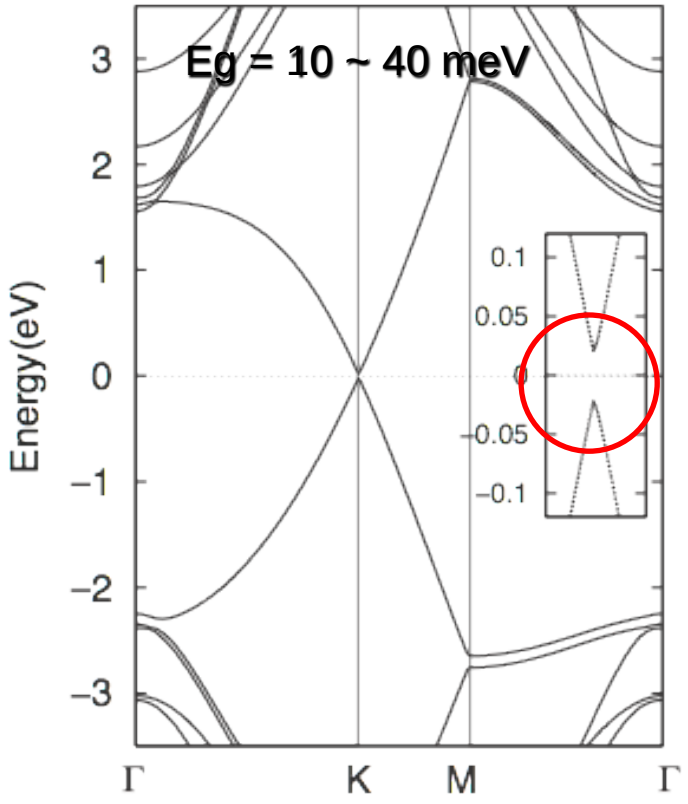
How graphene interacts with SiO_2, a typical base material of device?
First-principles density functional calculation is achieved.



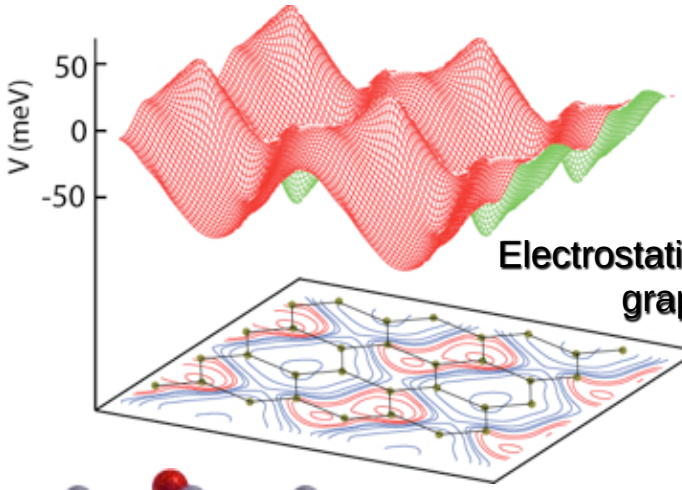
Electronic Structure of SiO_2 on Graphene

N. T. Cuong et al. Phys. Rev. Lett. 106, 106801 (2011)

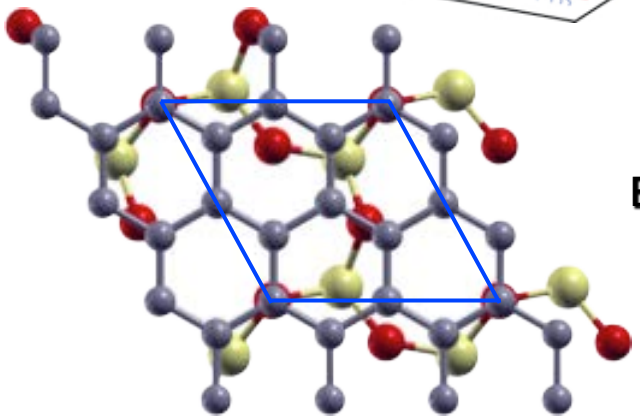
Originally metallic graphene gets small but finite bandgap by the interaction with SiO_2.



Finite energy gap



Electrostatic potential on graphene



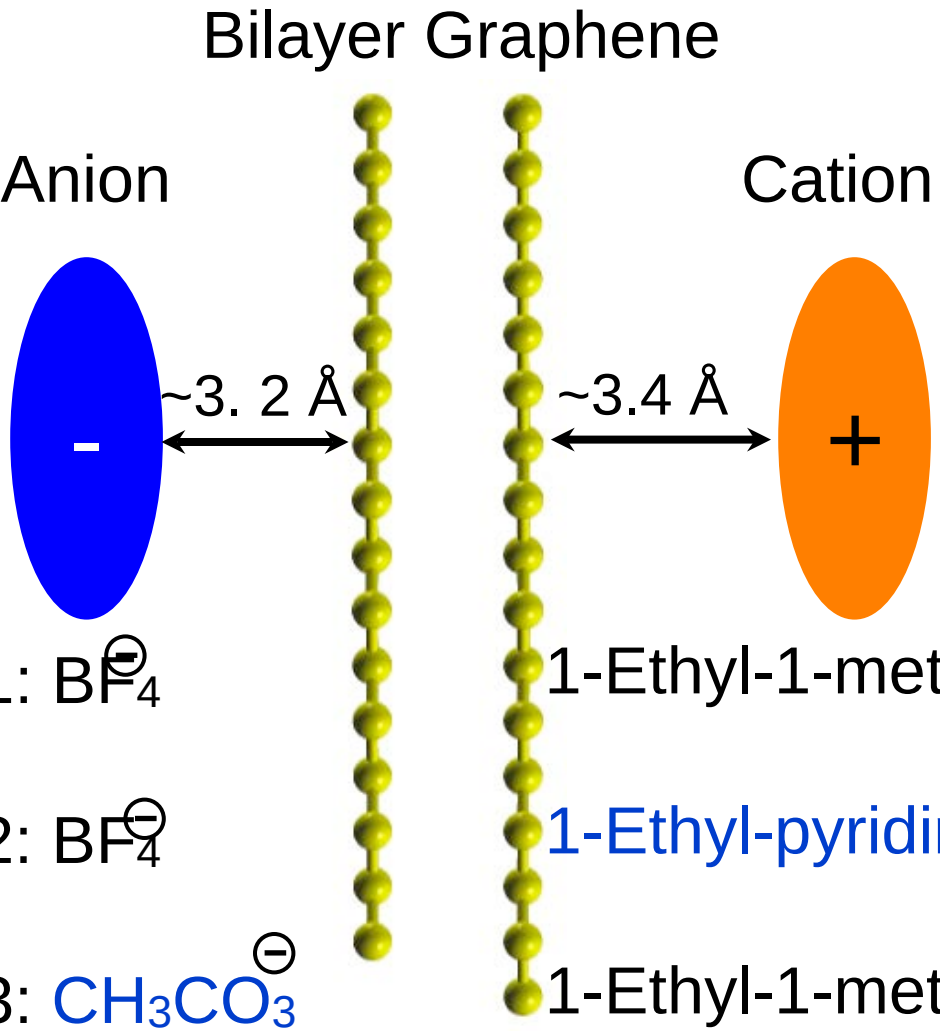
$E_{binding}$= 11.1 meV/C

$d_{Gra\text{-}SiO2}$ =2.88 Å

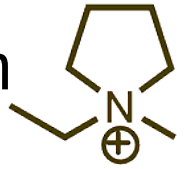
Structures of Graphene-Ionic Liq. Sandwich

Cuong, Appl. Phys. Lett. ('12)

Graphene is a metal. It is proposed to use the bilayer graphene as semiconductor device. How?

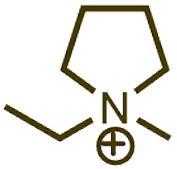


S1: BF_4^- 1-Ethyl-1-methyl-pyrrolidinium



S2: BF_4^- 1-Ethyl-pyridinium

S3: $CH_3CO_3^-$ 1-Ethyl-1-methyl-pyrrolidinium



Computational Optical Sciences

X.-M. Tong	Atoms and molecules under intense laser pulse
K. Yabana	Solids under intense laser pulse
N. Maeshima	Strongly correlated systems under light field

Laser-Matter interaction: Strong and Ultra-Short Laser Pulse

Strong light field

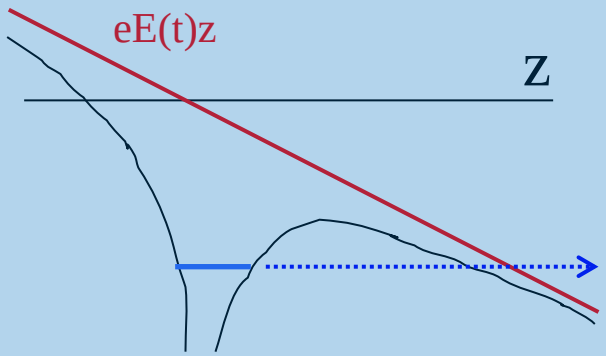
Magnitude of light electric field comparable to that bound electrons in matters.

Nonlinear, nonequilibrium Electron Dynamics

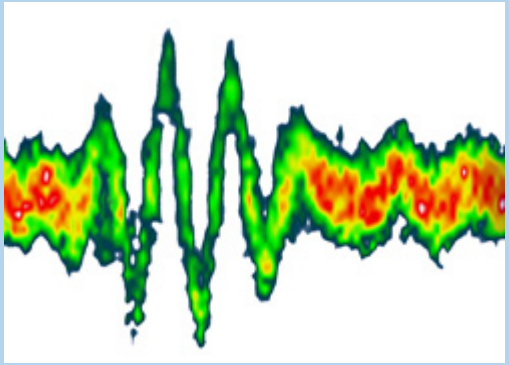
Ultra-short pulse

Pulse time duration comparable to a period of electron motion in matters.

Femto-technology
Atto-second science



Real-time observation of laser electric field using atto-second streaking technique

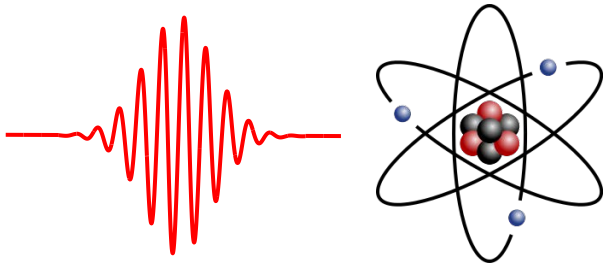


Joint LMU-MPQ Laboratory of Attosecond

X.-M. Tong

Atoms and molecules in strong laser pulse.

- Understand the mechanism of laser-matter interaction
- Control the dynamics in femtosecond (10^{-15} s) to attosecond (10^{-18} s) time scale.



Solve Time-Dependent Schrödinger Equation (TDSE) in real time and real space

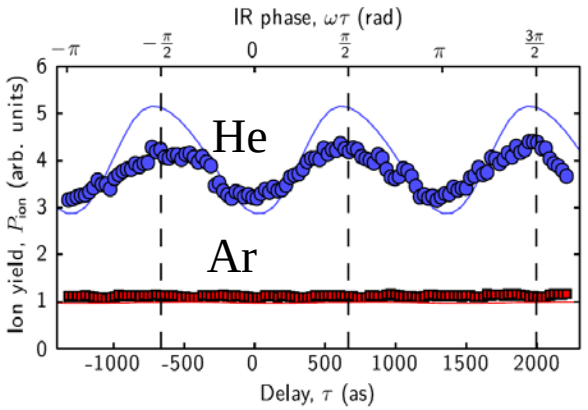
$$\left\{-\frac{\hbar^2}{2m}\vec{\nabla}^2-\frac{e^2}{r}+e\vec{E}(t)\cdot\vec{r}\right\}\psi_i(\vec{r},t)=i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)$$

- Split-operator method in energy representation
- Highly efficient calculation using BLAS, LAPACK, efficient implementation also in GPU clusters, HA-PACS

IR assisted atomic photoionization: Mechanism

Experiment observations: [PRL **99** (2007) 233001]

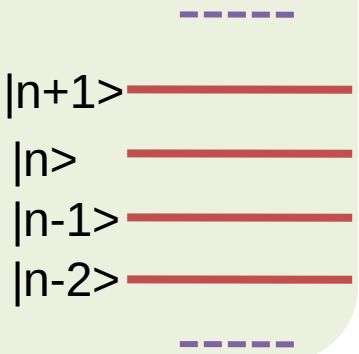
- He ionization yields oscillate
- Ar does not



Our proposed mechanism: [PRA 81 (2010) 021404(R)]

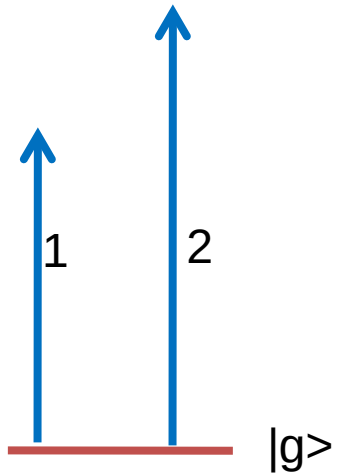
- Floquet states are formed by the IR field;
- XUV Excites atoms to a Floquet state *through different sidebands.*

$$\Psi_\alpha(\mathbf{r},t) = e^{-i\epsilon_\alpha t}\sum_{n=-\infty}^{\infty} e^{-i\ n\omega t}\phi_{\alpha,n}(\mathbf{r})$$



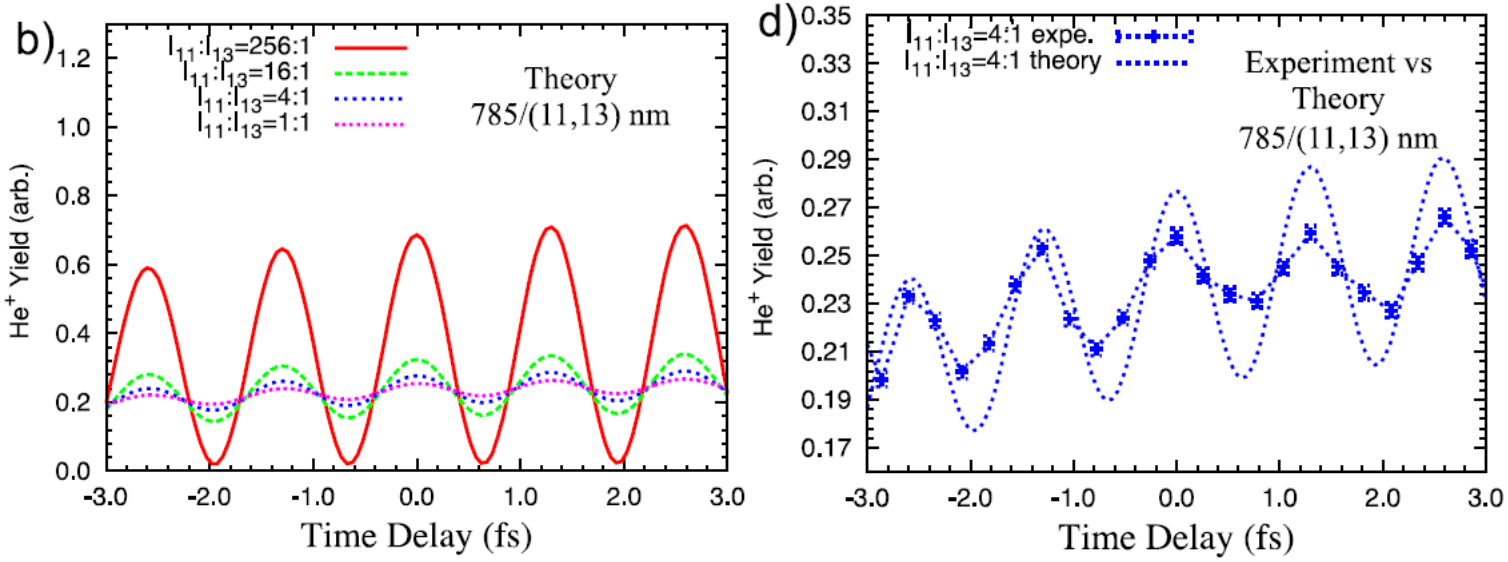
- The interference between the transition to different side bands results the oscillation.

$$P(t_d) \propto \sum_\alpha |M_1^\alpha F_1 + M_2^\alpha F_2\ e^{-i\ 2\omega t_d}|^2$$



Control atomic photoionization by IR fields

Tuning the arriving time to control the transparency. [PRL **106** (2011) 193008]



Other applications of the proposed theory

- Extract the emission time the Attosecond pulse PRA **85** (2013) 051802(R).
- Trace the time-evolution of a Laser-Dressed state PRL **108** (2012) 193002.
- Understand the abnormal intensity dependence PRA **81** (2010) 043429.

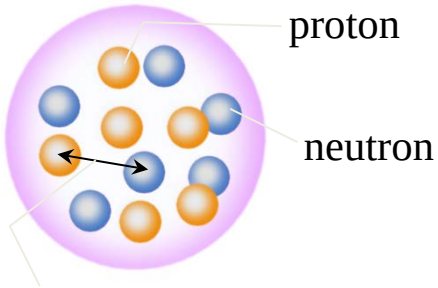
K. Yabana

Common method in two different systems:

Time-dependent Density Functional Theory (TDDFT)

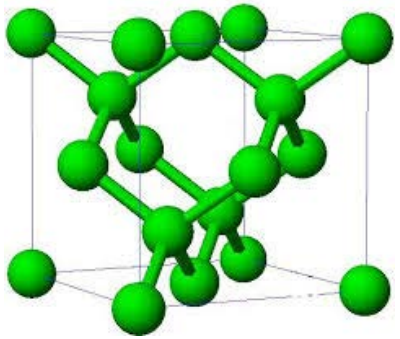
Nuclear Physics

Nucleon many-body system



Condensed Matter Physics

Electron many-body system



Solve time-dependent Kohn-Sham equation in real-time and real-space

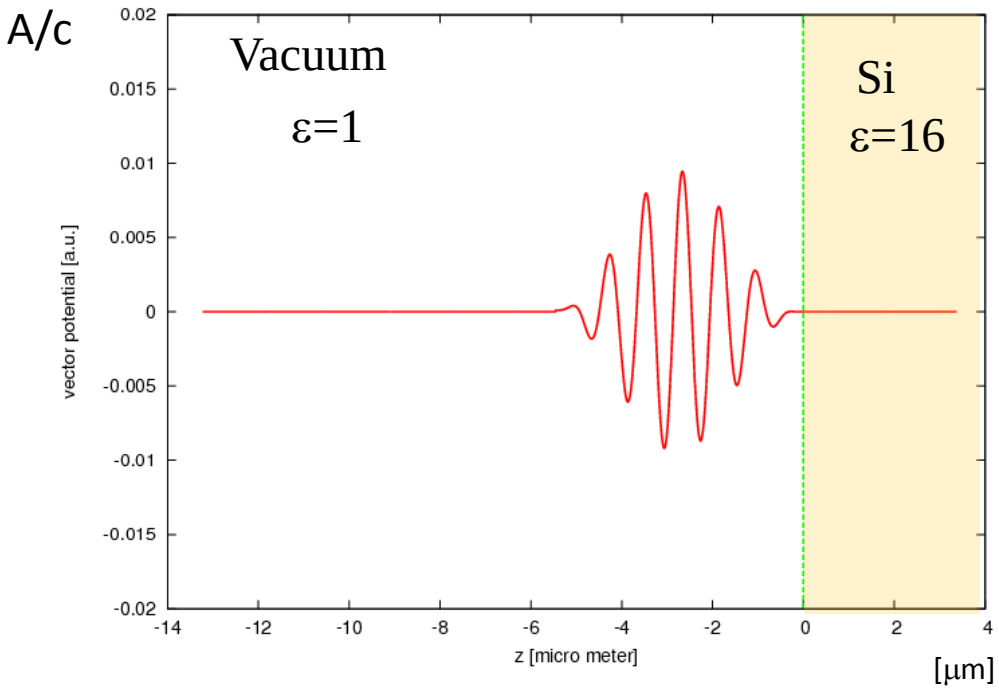
$$\left\{-\frac{\hbar^2}{2m}\vec{\nabla}^2+\sum_a V_{ion}(\vec{r}-\vec{R}_a)+e^2\int d\vec{r}\,'\frac{n(\vec{r}\,',t)}{|\vec{r}-\vec{r}\,'|}+\mu_{xc}(n(\vec{r},t))+V_{ext}(\vec{r},t)\right\}\psi_i(\vec{r},t)=i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t)$$

Research Highlight

First-principles calculation for laser - solid interaction

Femto- to Attosecond laser sciences

Question: How to describe strong laser pulse propagation in solids?



Usual situation

Macroscopic Maxwell equation. Electromagnetism is sufficient.

Extremely strong light field

Microscopically, strong electric field induce nonlinear electron dynamics.

How electromagnetism should be modified ?

Our answer.

Electromagnetism and quantum mechanics no more separate.

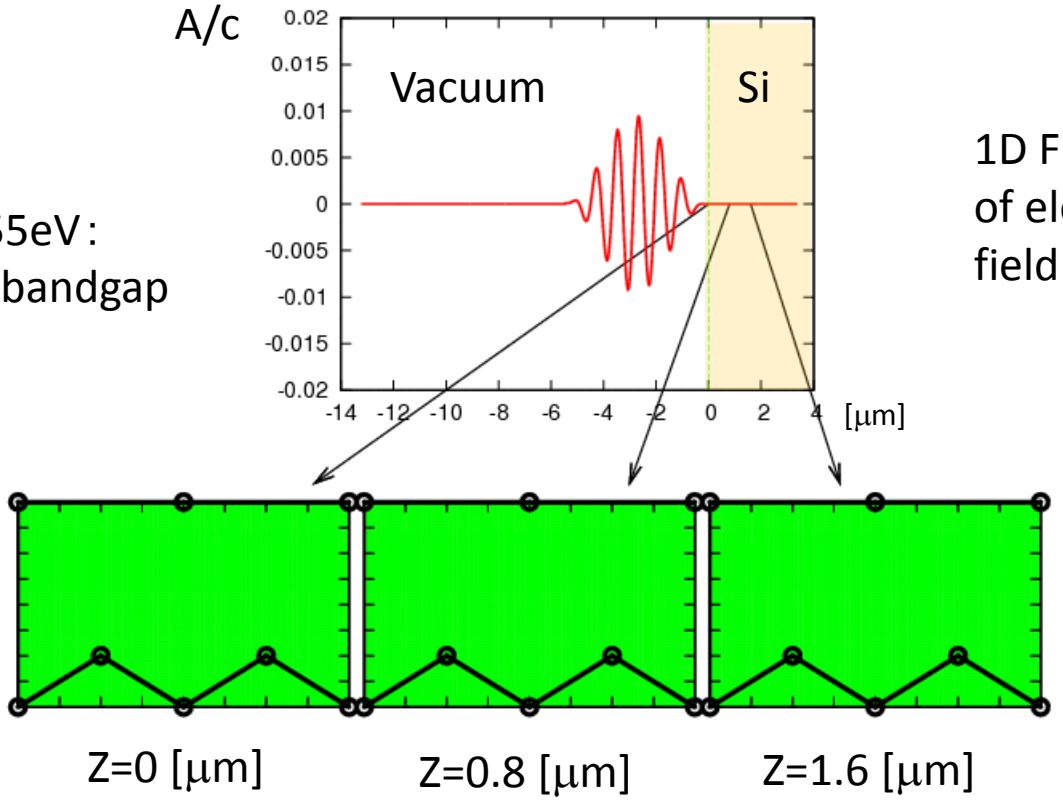
Need to couple two theories by large-scale computing.

Macroscpic electromagnetism + Microscopic electron dynamic

K. Yabana, T. Sugiyama, Y. Shinohara, T. Otobe, G.F. Bertsch, Phys. Rev. B85, 045134 (2012).

$I=10^{10}W/cm^2$

Laser frequency : 1.55eV :
lower than direct bandgap
2.4eV(LDA)



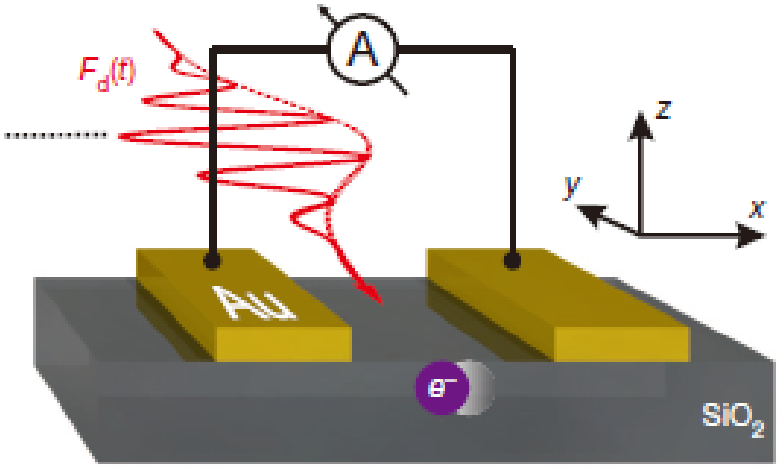
1D FDTD simulation of electromagnetic field

3D electron dynamics simulation by TDDFT

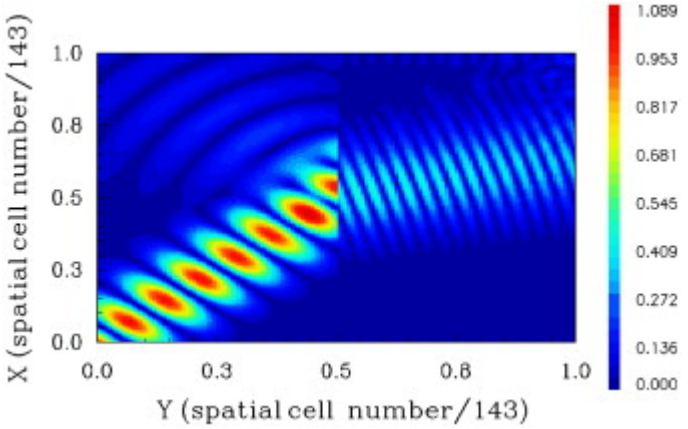
Coupled Maxwell + TDDFT simulation

Maxwell + TDDFT multiscale simulation will be useful in

Strong laser pulse on transparent glass induces ultrafast electric current



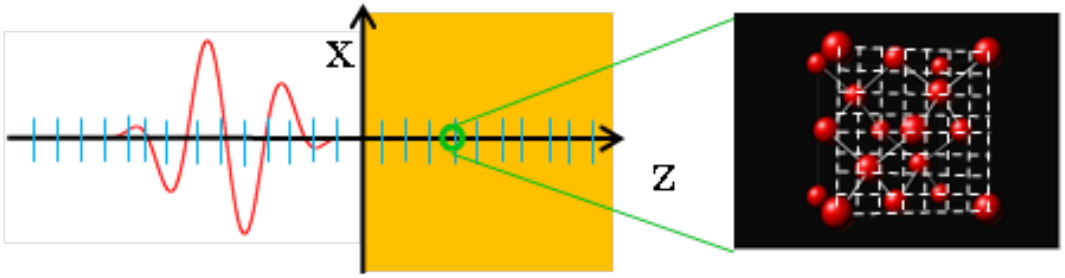
Basic question: what happens when Strong laser pulse irradiates in oblique angle?



Femtotechnology: nonthermal laser machinery

Figure B1 Femtosecond laser micromaching process. **a**, Schematic of the laser incident on a transparent material. **b**, Diagram of the excitation of electrons to the conduction band. **c**, Microscope images showing the large variation in the feature characteristics depending on the experimental conditions. Left: single 10-nJ pulse and right: 25,000 5-nJ pulses at a frequency of 25 MHz (both with the same focal spot).

Maxwell + TDDFT simulation requires large computer resources

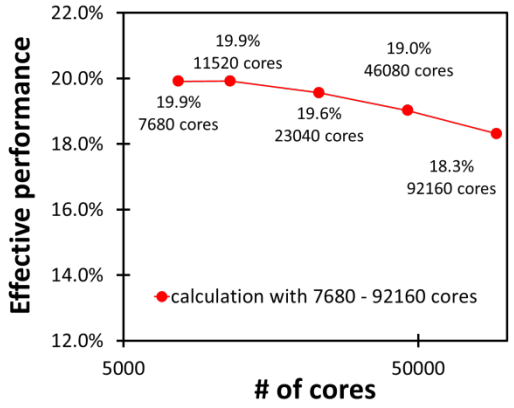


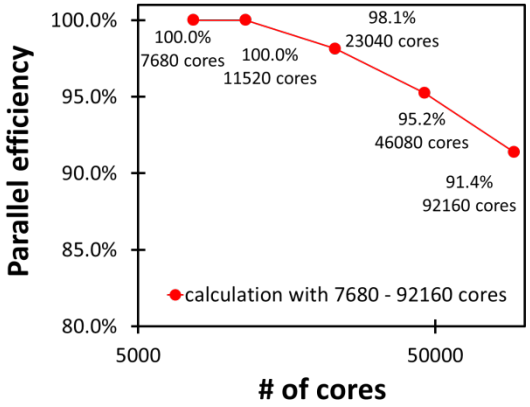
Si, diamond:

1,000 cores, 10 hours

SiO_2 (α-quartz)

10,000 cores, 6 hours (at K-computer)





Good performance up to 100,000 cores.

We expect to carry out calculations in K-computer through strategic use as well as general use.

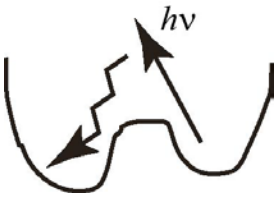
N. Maeshima

Strongly correlated systems under light field

Photo-induced ”phase transition”

- **Photo excitation → phase transition**

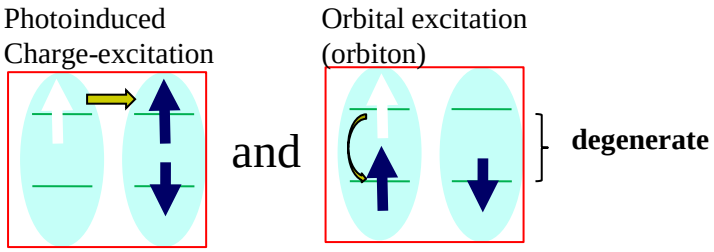
  Stable ⇔ Metastable



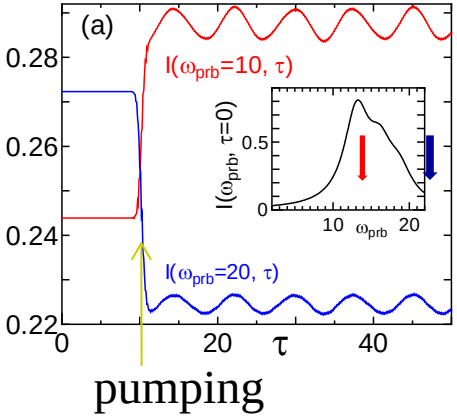
- **Quantum dynamics**
  - **photoinduced ultra-fast coherent oscillation**
- **Effect of electron-lattice interaction**
  - **photoinduced absorption 1D organic insulators**

Photoinduced coherent oscillation in orbital degenerate systems

Photoinduced dynamics in orbital degenerated systems and related excitations



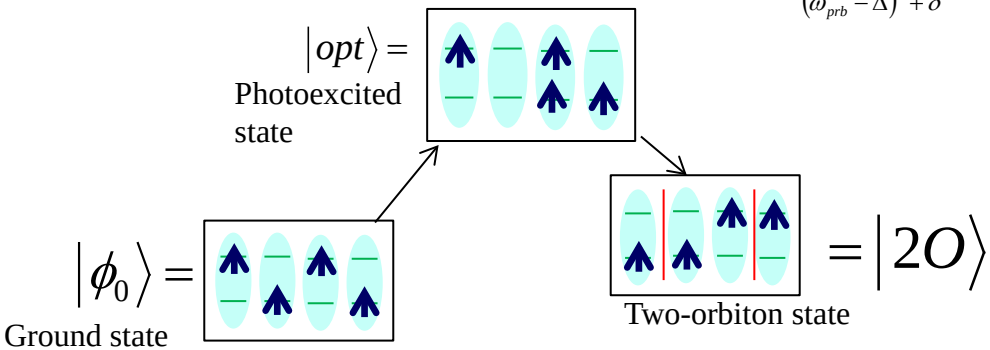
transient optical response function of 1D two-orbital degenerate Hubbard model



dominant oscillating component

$$I(\omega_{prb},\tau) \approx \langle 2O \mid j \mid opt\rangle\langle opt \mid j \mid \phi_0\rangle e^{i(\varepsilon_{2O}-\varepsilon_0)\tau} f_L[\omega_{prb}-(\varepsilon_{opt}-\varepsilon_0)] + c.c.$$

$$f_L[\omega_{prb}-\Delta] = \frac{\delta}{(\omega_{prb}-\Delta)^2+\delta^2}$$



Quantum coherence between the ground state and the two-orbiton state

Pump-probe experiment

D. Polli, M. Rini, S. Wall, R. W. Schoenlein, Y. Tomioka, Y. Tokura, G. Cerullo, and A. Cavalleri, Nature Mater. **6**, 643 (2007).

References

N. Maeshima, K. Hino, and K. Yonemitsu, Phys. Rev. B **82**, 161105(R) (2010)

N. Maeshima, K. Hino, and K. Yonemitsu, Physica Status Solidi (c) **8**, 213 (2011)

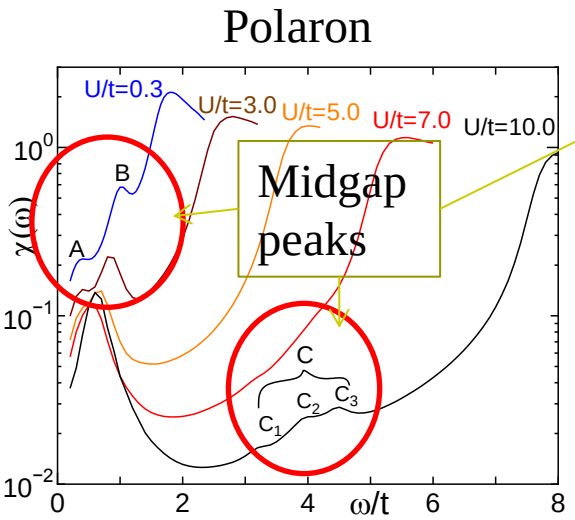
photoinduced absorption of 1D organic insulators

Carrier + lattice relaxation in 1D Peierls-Hubbard model

$$H = -\sum_{l,\sigma}(t-u_l)(c^{\dagger}_{l\sigma}c_{l+1\sigma}+H.c.)+U\sum_{l}n_{l\uparrow}n_{l\downarrow}$$

$$+\frac{K_\alpha}{2}\sum_{l}u_l^2$$

Optical response (numerical calculation)



Pump-probe experiment (K-TCNQ)

H. Okamoto *et al.*, *PRL*. **96,** 037405 (2006)

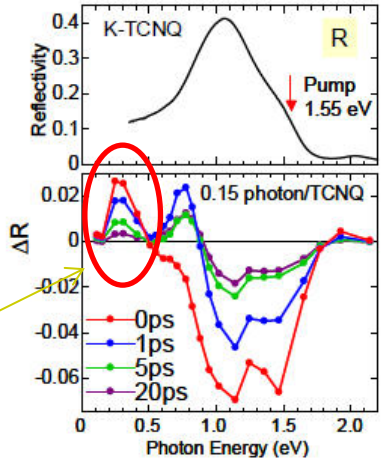
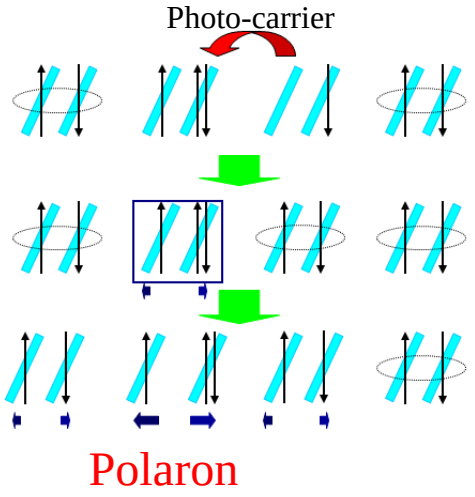


Photo-excitation and formation of polaron



references

N. Maeshima, K. Moriya, and K. Hino, J. Phys. Soc. Jpn. **81**, 104708_1-7 (2012)

H. Uemura, N. Maeshima, K. Yonemitsu, and H. Okamoto, Phys. Rev. B **85**, 125112_1-7 (2012)

N. Maeshima and K. Yonemitsu, J. Phys. Soc. Jpn. **77**, 074713_1-6, (2008

Strongly Correlated Systems

H. Koizumi

1. The elucidation of the mechanism of the high temperature superconductivity in the cuprates
2. Theoretical study for the realization of the quantum computer using the cuprate

The understanding of the mechanism of high temperature superconductivity in cuprates.

1. Key to the room temperature superconductivity: a desired technology for environmentally friendly human society.

2. Understanding for the novel electronic state due to the interplay between spin and charge degrees of electrons: spintronics application.

3. Macroscopic quantum phenomena above the boiling temperature of nitrogen: realization of quantum computers near or above the room temperature.

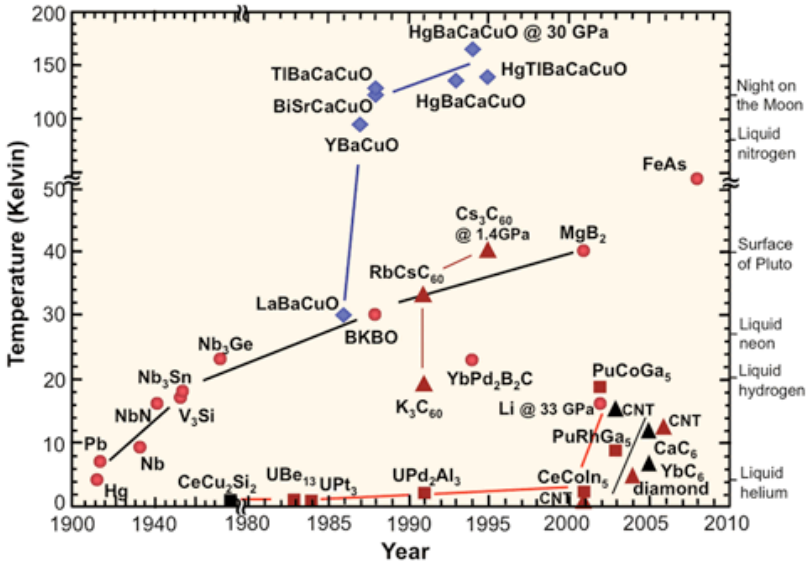
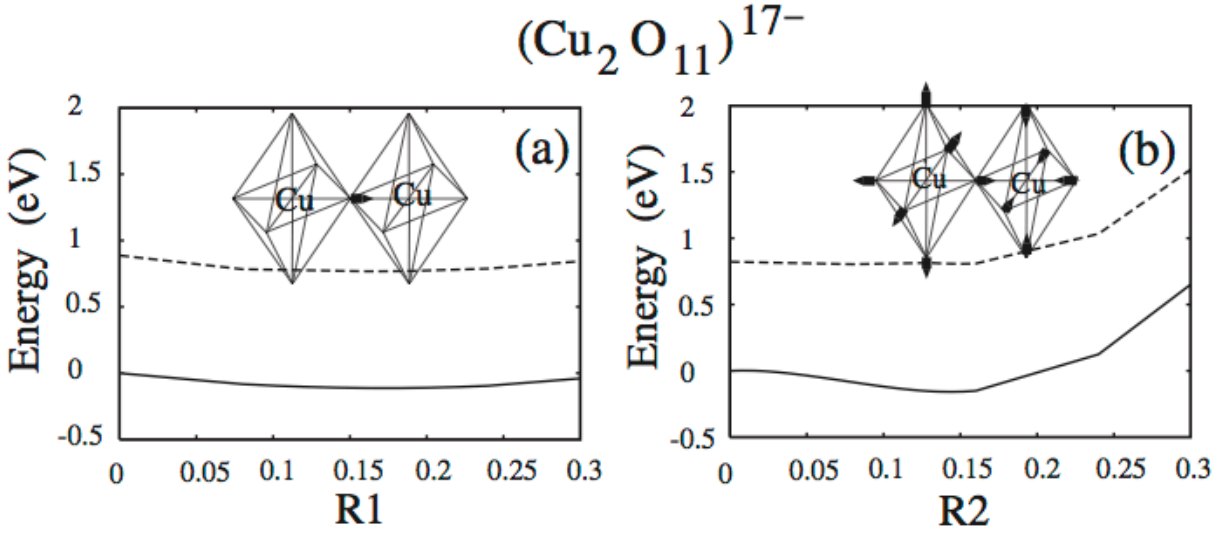


Figure: the highest superconducting transition temperature T_c v.s. year. The Tc jumped up at 1986 when the cuprate was discovered; only cuprates have Tc above the boiling temperature of nitrogen.

Ab initio molecular orbital cluster calculation has revealed that the doped holes become small polarons in the bulk.
The Cu-O bond length change agrees with the value observed by EXFAS experiment.

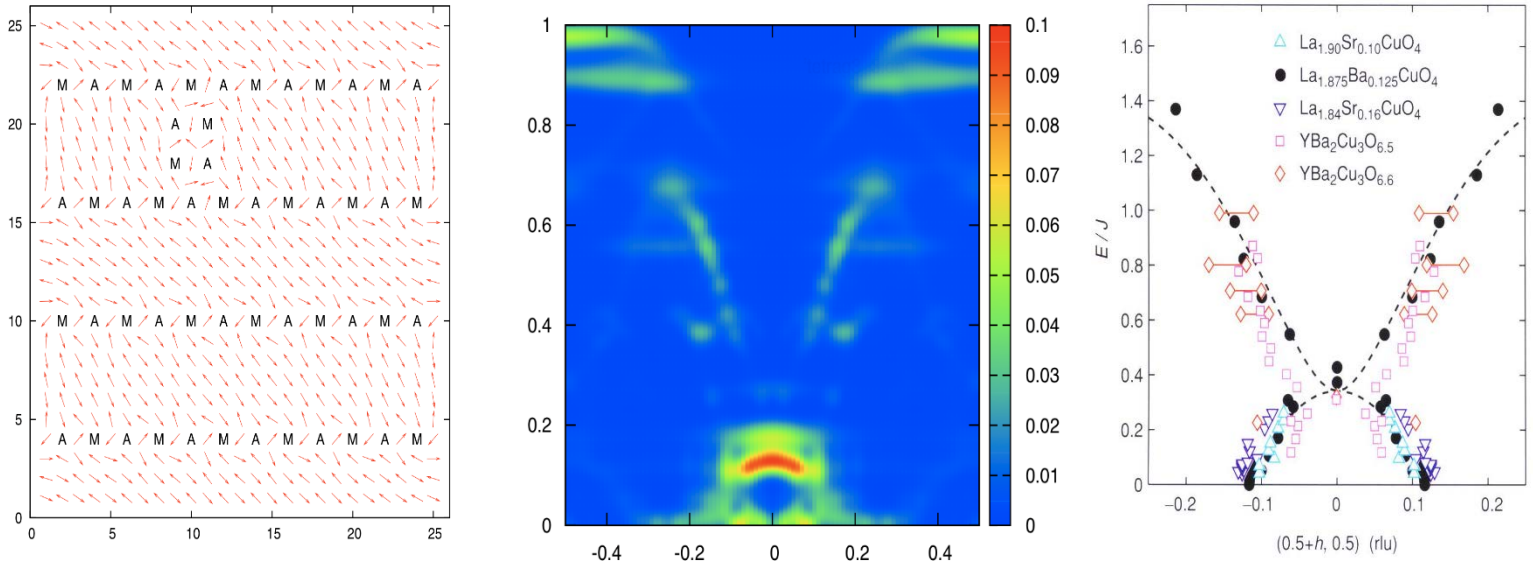


S. Miyaki, K. Makoshi, H. Koizumi, Two-Copper-Atom Units Induce a Pseudo Jahn-Teller Polaron in Hole-Doped Cuprate Superconductors, J. Phys. Soc. Jpn. 77, 034702-1-6, (2008)

Spin-wave spectrum calculated by the Heisenberg model with spin-vortices embedded in the antierromagnetic background yields the magnetic excitation specrum observed by the neutron scattering experiment.

H. Koizumi, Spin-wave excitations in effectively half-filled Mott insulators, J. Phys. Soc. Jpn., 104704-1-10, (2008)

R. Hidekata, H. Koizumi, Spin-vortices and spin-vortex-induced loop currents in the pseudogap phase of cuprates, J. Supercond. Nov. Magn. 24, 2253-2267, (2011)



Left: A spin configuration with spin-vortices embedded in an antiferromagnetic arrangement.
Middle: Spin wave excitation spectrum calculated with the left spin configuration.
Right: Experimentally obtained magnetic excitation spectrum.

Spin-vortex-induced loop current

We predict spin-vortices generated by itinerant electrons induce loop currents. They will exist in the CuO_2 plane in the cuprate.

H. Koizumi, R. Hidekata, A. Okazaki, M. Tachiki, Persistent current generation by the spin-vortex formation in cuprate with the single-valuedness constraint on the conduction electron wave functions, to appear in *J. Supercond. Nov. Magn.* DOI 10.1007/s10948-013-2277-2 (2013)

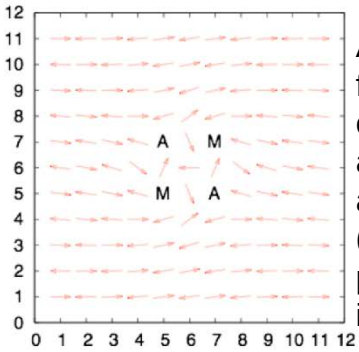
$$\mathbf{j}(\mathbf{x}) = \frac{2q}{\hbar} \sum_{\ell=1}^{N_{loop}} \lambda_\ell \frac{\delta}{\delta \nabla \chi(\mathbf{x})} \oint_{C_\ell} \nabla \chi(\mathbf{y}) \cdot d\mathbf{y}$$

N_{loop} : The number of independent loops

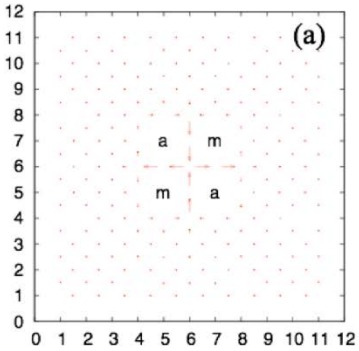
q : charge on electron, q = –e

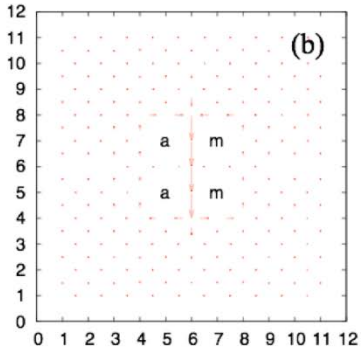
χ : London's superpotential, angular vaLriable with period 2π

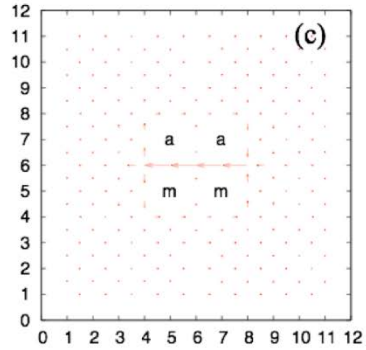
λ_ℓ : The Lagrange multiplier for the single - valued constraint of wave functions

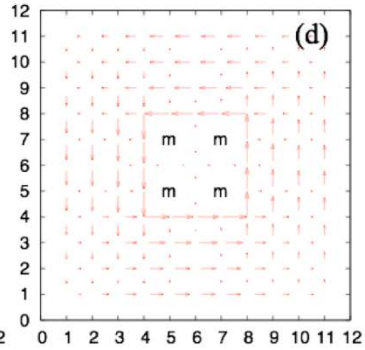


A spin configuration with four spin-vortices embedded in the antiferromagnetic spin arrangement.
(a)-(d): four different patterns of spin-vortex-induced loop currents









Summary

Computational Nano-Sciences:

- Successful collaboration between physicists and computer scientists to produce RSDFT code, which won the Gordon Bell Prize 2011.
- Due to members' move, group is under reconstruction.

Computational Optical Sciences:

- Focusing on time-dependent electron dynamics simulation which is developing as an emerging important field of computational physics

Strongly-Correlated Systems:

- Important area where first-principles method cannot be applied.